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Key indicators

Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.051
 wR factor = 0.115
Data-to-parameter ratio = 12.5

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

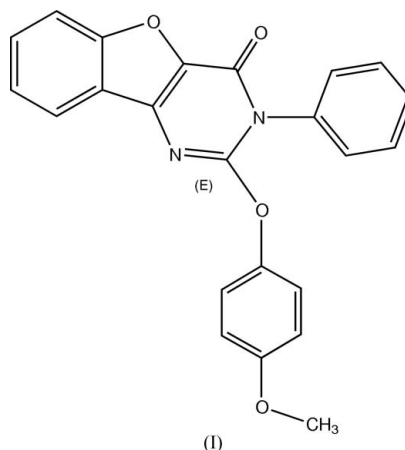
3-(4-Methoxyphenoxy)-2-phenyl-3*H*-1-benzofuro[3,2-*d*]pyrimidin-1-one

In the title compound, $\text{C}_{23}\text{H}_{16}\text{N}_2\text{O}_4$, the molecules form a supramolecular structure *via* intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and intermolecular $\pi-\pi$ interactions.

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Comment

Pyrimidine derivatives are attracting increasing attention in the synthetic chemistry community because of the important role played by such systems in many natural products, antibiotics and drugs (Ding *et al.*, 2004). In recent years, we have been engaged in the preparation of derivatives of heterocycles using the aza-Wittig reaction. In this paper, we present the X-ray crystallographic analysis of the title compound, (I).



The structure of (I) is shown in Fig. 1, and selected bond lengths and angles are listed in Table 1. All ring atoms in the benzofuro[3,2-*d*]pyrimidine system are essentially coplanar.

A number of weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions are present. Atom O3 and atom H23C on atom C23 of the neighbouring OCH_3 group form a weak $\text{C}-\text{H}\cdots\text{O}$ interaction (Table 2). The symmetry-imposed dihedral angle between two aromatic rings (atoms C17–C22) of adjacent molecules is 0° and the distance between ring centroids is $3.852(1)$ Å, showing that $\pi-\pi$ stacking interactions are present (Janiak, 2000).

Experimental

To a solution of *N*-(2-ethoxycarbonylbenzofuran-3-yl)iminotriphenylphosphorane (3 mmol) in dry methylene dichloride (15 ml) was added aromatic isocyanate (3 mmol) under nitrogen at room temperature. After the reaction mixture had been allowed to stand for 10 h at 273–278 K, the solvent was removed off under reduced pressure and ether/petroleum ether (1:2 *v/v*, 20 ml) was added to precipitate triphenylphosphine oxide. After filtration, the solvent was removed to give the carbodiimide, which was used directly without

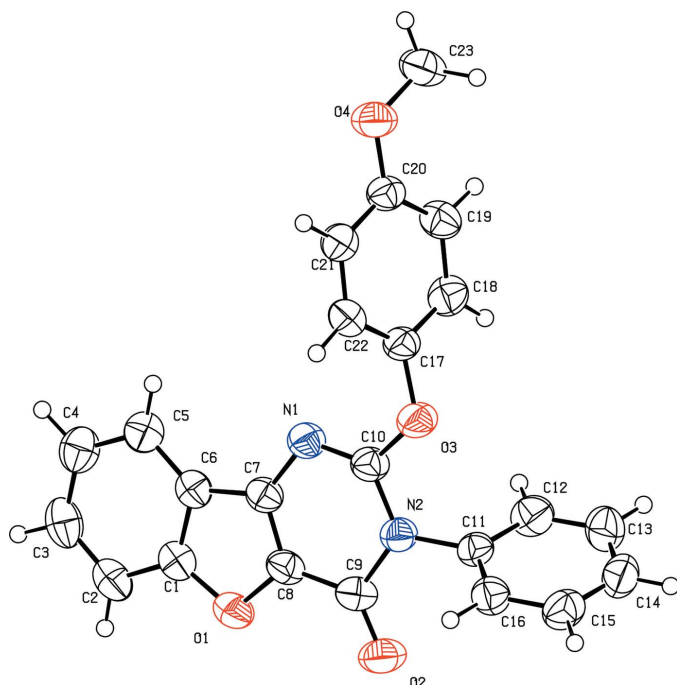


Figure 1
A view of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

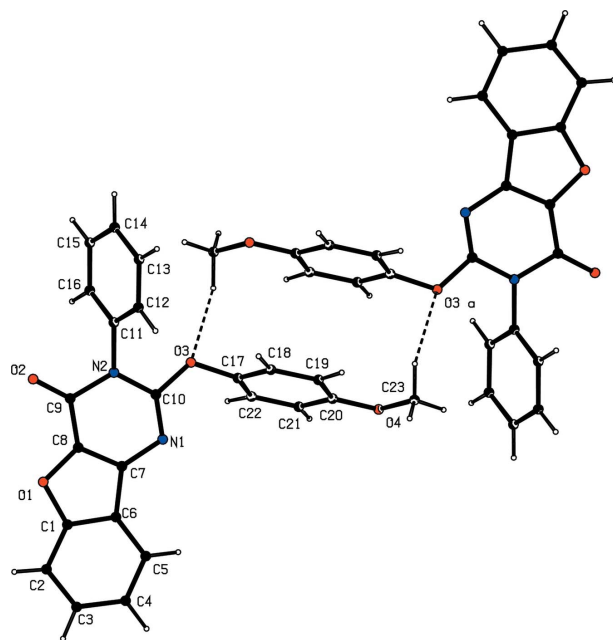


Figure 2
Two molecules of (I), showing the formation of the C—H...O hydrogen bonds and the π - π stacking interactions [symmetry code: (a) $-x + 1, -y + 1, -z + 2$].

further purification. To a solution of carbodiimide in acetonitrile (15 ml) were added 4-methoxyphenol (3 mmol) and anhydrous K_2CO_3 (1 mmol). The mixture was stirred for 6 h at 313–318 K. The solution was concentrated under reduced pressure and the residue was recrystallized from methylene dichloride and ethanol to give the title compound, (I). Suitable crystals were obtained by vapour diffusion of ethanol at room temperature. Elemental analysis calcu-

lated for $C_{23}H_{16}N_2O_4$: C 71.87, H 4.17, N 7.29%; found: C 71.80, H 4.23, N 7.35%.

Crystal data

$C_{23}H_{16}N_2O_4$
 $M_r = 384.38$
Monoclinic, $P2_1/c$
 $a = 9.3415$ (12) Å
 $b = 10.0584$ (12) Å
 $c = 19.976$ (3) Å
 $\beta = 92.262$ (2)°
 $V = 1875.5$ (4) Å³
 $Z = 4$

$D_x = 1.361$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 1839 reflections
 $\theta = 2.2$ – 21.6 °
 $\mu = 0.10$ mm⁻¹
 $T = 292$ (2) K
Needle, colourless
 $0.55 \times 0.20 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
Absorption correction: none
10770 measured reflections
4082 independent reflections

2620 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.042$
 $\theta_{max} = 27.0$ °
 $h = -11 \rightarrow 11$
 $k = -12 \rightarrow 10$
 $l = -25 \rightarrow 23$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.115$
 $S = 1.02$
4082 reflections
326 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 0.0501P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.13$ e Å⁻³
 $\Delta\rho_{min} = -0.18$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

C1—C2	1.380 (3)	C9—N2	1.426 (2)
C1—C6	1.389 (2)	C10—N1	1.287 (2)
C1—O1	1.392 (2)	C10—O3	1.341 (2)
C4—C5	1.370 (3)	C11—N2	1.451 (2)
C6—C7	1.434 (2)	C17—O3	1.409 (2)
C7—N1	1.376 (2)	C20—O4	1.366 (2)
C8—O1	1.379 (2)	C23—O4	1.430 (3)
C9—O2	1.220 (2)		
C2—C1—C6	123.7 (2)	C12—C11—N2	119.96 (17)
C6—C1—O1	111.39 (16)	C18—C17—O3	116.99 (17)
C5—C6—C7	135.76 (18)	C22—C17—O3	121.44 (18)
C8—C7—N1	123.80 (17)	O4—C20—C19	124.30 (18)
C7—C8—O1	112.51 (16)	C10—N2—C9	121.79 (15)
O1—C8—C9	123.39 (16)	C8—O1—C1	104.26 (14)
O2—C9—N2	121.79 (18)	C10—O3—C17	119.65 (14)
N1—C10—O3	121.88 (16)	C20—O4—C23	117.37 (18)
N1—C10—N2	127.16 (17)		
C6—C1—C2—C3	0.5 (3)	C17—C18—C19—C20	-0.3 (3)
O1—C1—C2—C3	-179.80 (17)	O4—C20—C21—C22	-179.04 (18)
C3—C4—C5—C6	-0.6 (3)	C6—C7—N1—C10	-175.86 (18)
C1—C6—C7—N1	-179.80 (18)	O3—C10—N2—C11	-9.5 (2)
N1—C7—C8—O1	179.74 (16)	O2—C9—N2—C10	179.01 (17)
C7—C8—C9—O2	-173.48 (19)	C6—C1—O1—C8	0.1 (2)
O1—C8—C9—N2	176.54 (16)	C19—C20—O4—C23	-0.8 (3)
N2—C11—C16—C15	-179.87 (17)	C21—C20—O4—C23	178.07 (19)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C23—H23C...O3 ⁱ	1.04 (2)	2.48 (2)	3.312 (3)	136 (2)

Symmetry code: (i) $-x + 1, -y + 1, -z + 2$.

All H atoms were refined freely, with C–H distances in the range 0.91 (2)–1.00 (2) Å.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL*.

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